Simulation of Turbulent Premixed Combustion

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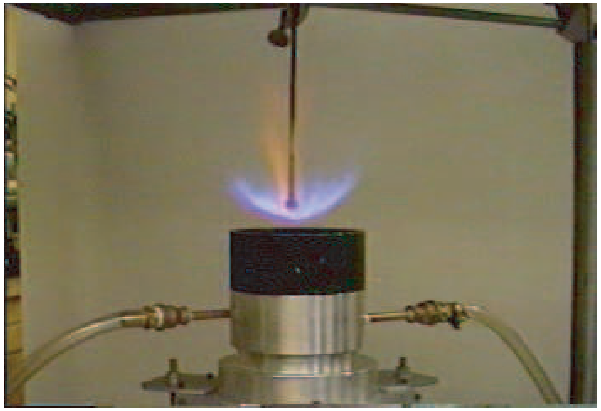
Objective

Simulate laboratory-scale turbulent premixed combustion using detailed kinetics and transport without subgrid models for turbulence or turbulence-chemistry interaction

Premixed Low-Swirl Burner



Application:

Fundamental studies of turbulent flame dynamics

Pollutant (NO_x) formation in turbulent laboratory flame

Rod-stabilized Flame

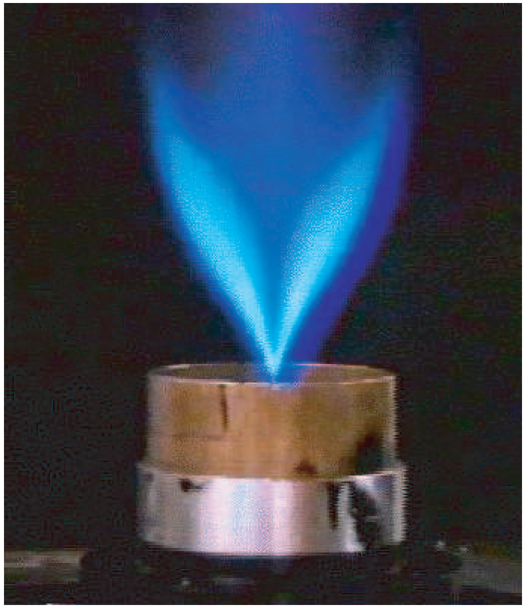


Photo courtesy R. Cheng

Traditional approach:

Compressible DNS

- High-order explicit finite-difference methods
- At least $O(10^9)$ zones
- At least $O(10^6)$ timesteps

Approach

With traditional methods, laboratory-scale simulations with detailed chemistry and transport are intractable for the near future

Observation:

- Laboratory turbulent flames are low Mach number
- Regions requiring high-resolution are localized in space

Our approach:

- Low Mach number formulation
  - Eliminate acoustic time-step restriction while retaining compressibility effects due to heat release
  - Conserve species and enthalpy
- Adaptive mesh refinement
  - Localize mesh where needed
  - Complexity from synchronization of elliptic solves
- Parallel architectures
  - Distributed memory implementation using BoxLib framework
  - Dynamic load balancing
  - Heterogeneous work load

Low Mach Number Combustion

Low Mach number model, $M = U/c \ll 1$ (Rehm & Baum 1978, Majda & Sethian 1985)

$$p(\vec{x},t) = p_0(t) + \pi(\vec{x},t) \quad \text{where} \quad \pi/p_0 \sim \mathcal{O}(M^2)$$

- p_0 does not affect local dynamics, π does not affect thermodynamics
- Acoustic waves analytically removed (or, have been “relaxed” away)
- $\vec{U}$ satisfies a divergence constraint, $\nabla \cdot \vec{U} = S$

Conservation equations:

$$\rho \frac{D\vec{U}}{Dt} + \nabla\pi = \nabla \cdot \tau$$

$$\frac{\partial \rho Y_\ell}{\partial t} + \nabla \cdot \left(\rho Y_\ell \vec{U}\right) = \nabla \cdot \vec{F}_\ell + \rho\dot{\omega}_\ell$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot \left(\rho h \vec{U}\right) = \nabla \cdot \vec{Q}$$

- Y_ℓ mass fraction
- $\vec{F}_\ell$ species diffusion, $\sum \vec{F}_\ell = 0$
- $\dot{\omega}_\ell$ species production, $\sum \dot{\omega}_\ell = 0$
- h enthalpy $h = \sum Y_\ell h_\ell(T)$
- $\vec{Q}$ heat flux
- $p = \rho R T \sum Y_\ell / W_\ell$

Fractional Step Approach

1. Advance velocity from $\vec{U}^n$ to $\vec{U}^{n+1,*}$ using explicit advection terms, semi-implicit diffusion terms, and a lagged pressure gradient.
2. Update the species, enthalpy and temperature, using explicit advection terms, semi-implicit diffusion terms, and source terms from stiff ODE integrators. Use the updated values to compute S^{n+1}
3. Decompose $\vec{U}^{n+1,*}$ to extract the component satisfying the divergence constraint.

This decomposition is achieved by solving

$$\nabla \cdot \left(\frac{1}{\rho} \nabla \phi \right) = \nabla \cdot \vec{U}^{n+1,*} - S^{n+1}$$

for ϕ, and setting

$$p^{n+1/2} = p^{n-1/2} + \phi$$

and

$$\vec{U}^{n+1} = \vec{U}^{n+1,*} - \frac{1}{\rho} \nabla \phi$$

Properties of the methodology

Overall operator-split projection formulation is 2^{nd}-order accurate in space and time.

Godunov-type discretization of advection terms provides a robust 2^{nd}-order accurate treatment of advective transport.

Formulation conserves species, mass and energy.

Equation of state is only approximately satisfied

$$p_o \neq \rho R T \sum_m \frac{Y_m}{W_m}$$

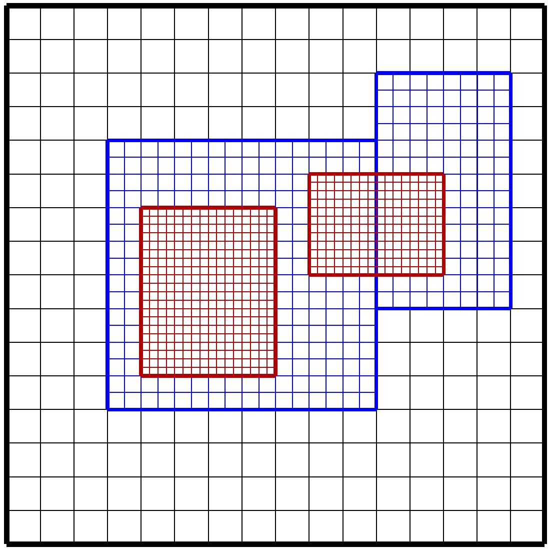
but modified constraint minimizes drift from equation of state.

AMR - Grid Structure

Block-structured hierarchical grids

Each grid patch (2D or 3D)

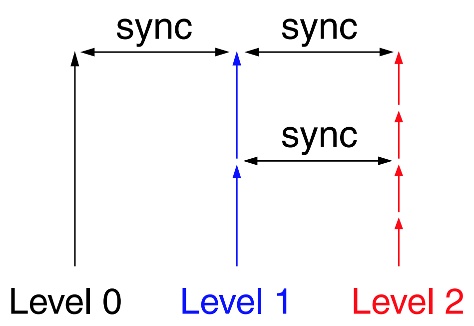
- Logically structured, rectangular
- Refined in space and time by evenly dividing coarse grid cells
- Dynamically created/destroyed to track time-dependent features



2D adaptive grid hierarchy

Subcycling:

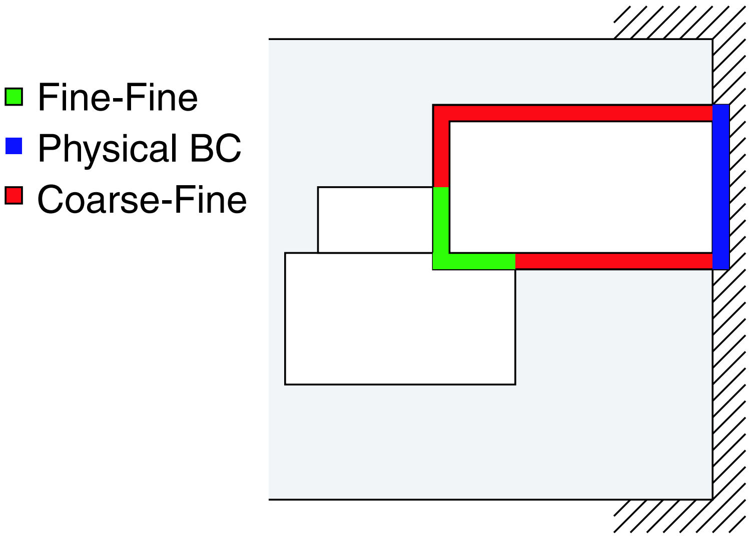
- Advance level ℓ, then
  - Advance level $\ell + 1$
    level ℓ supplies boundary data
  - Synchronize levels ℓ and $\ell + 1$

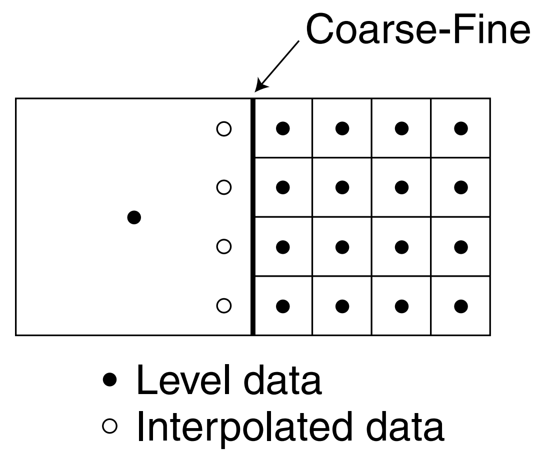


Preserves properties of single-grid algorithm

AMR level operations

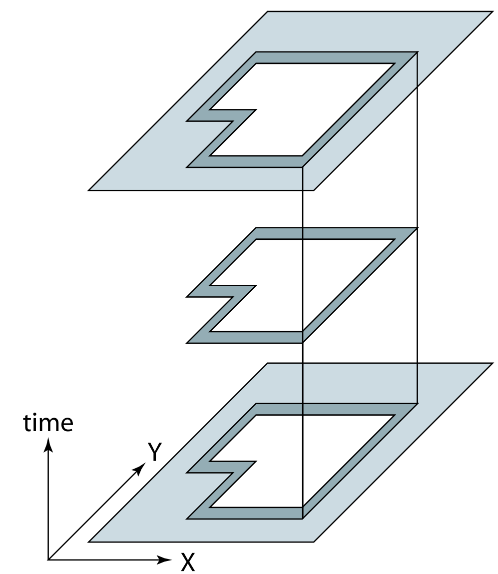
Organize grids by refinement level, couple through “ghost” cells





On the coarse-fine interface:

- Fine: Boundary cells filled from coarse data
  - Interpolated in space and time
- Coarse: Incorporate improved fine solution
  - “Synchronization”



Dynamic Load-Balancing

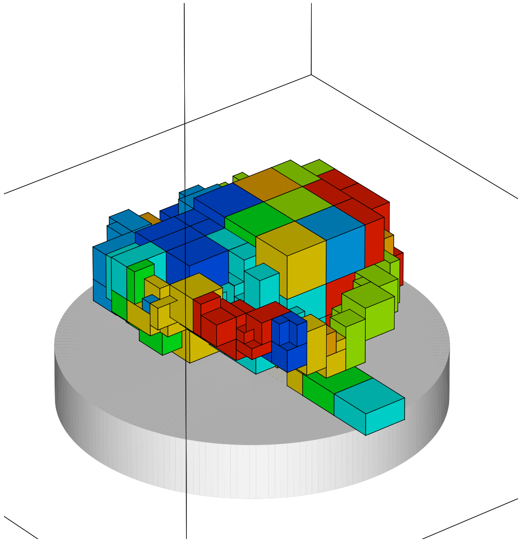
Approach: Estimate work per grid, distribute using heuristic KNAPSACK algorithm

Cells/grid often a good work estimate, but chemical kinetics may be highly variable

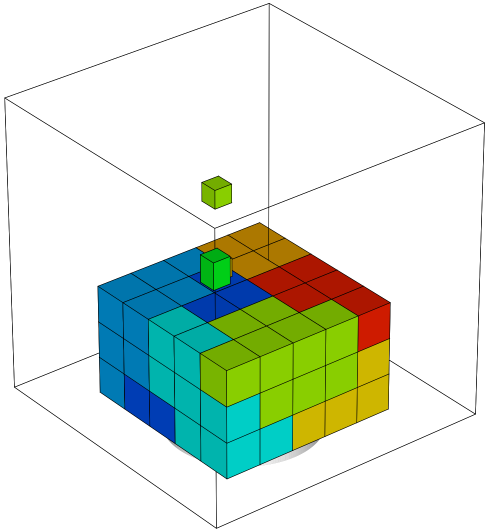
- Monitor chemistry integration work
- Distribute chemistry work based on this work estimate

Parallel Communication: AMR data communication patterns are complex

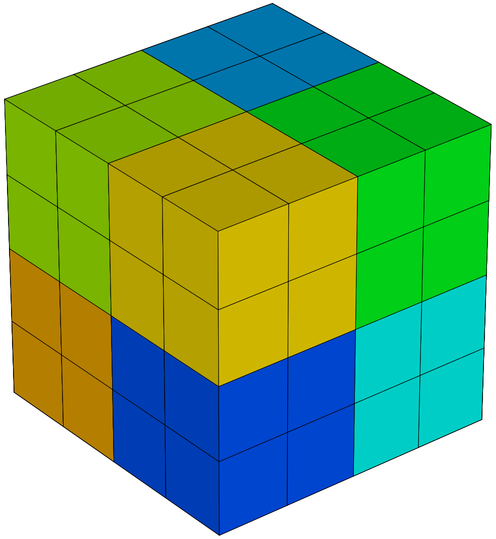
- Easy: distribute grids at a single level, minimize off-processor communication
- Hard: Incorporate coarse-fine interpolation (also, “recursive” interpolation)



Level 2



Level 1



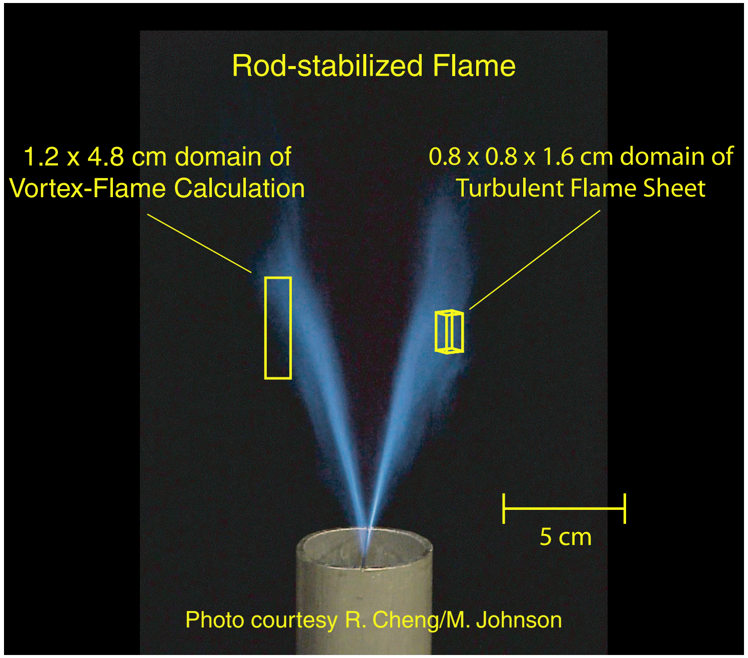
Level 0

Model problems

2-D Vortex flame interactions

(28th International Combustion Sympsium, 2000)

- 1.2 $\times$ 4.8 mm domain
- 53 species, 325 reactions



3-D Turbulent flame sheet

(29th International Combustion Sympsium, 2002)

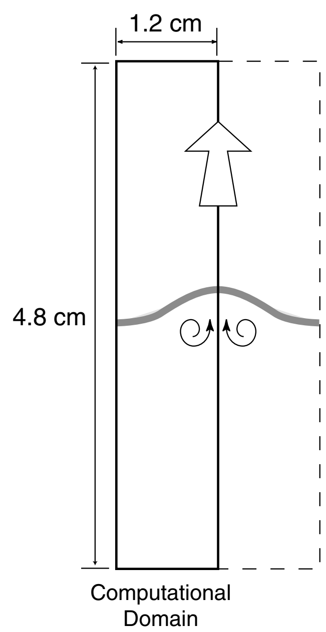
- .8 $\times$ .8 $\times$ 1.6 cm domain
- 21 species, 84 reactions

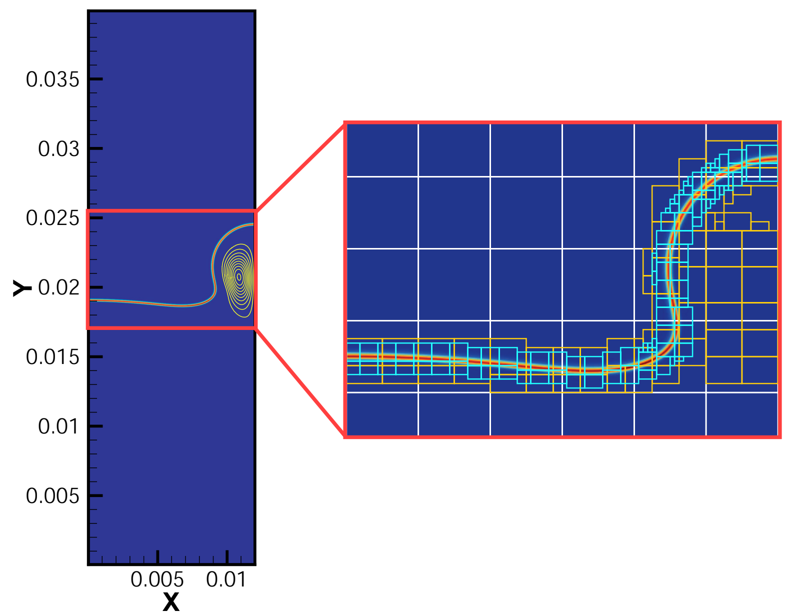
Laboratory-scale V-flame

(19th International Colloquium on the Dynamics of Explosions and Reactive Systems, 2003)

- 12 $\times$ 12 $\times$ 12 cm domain
- 21 species, 84 reactions

Vortex flame interaction

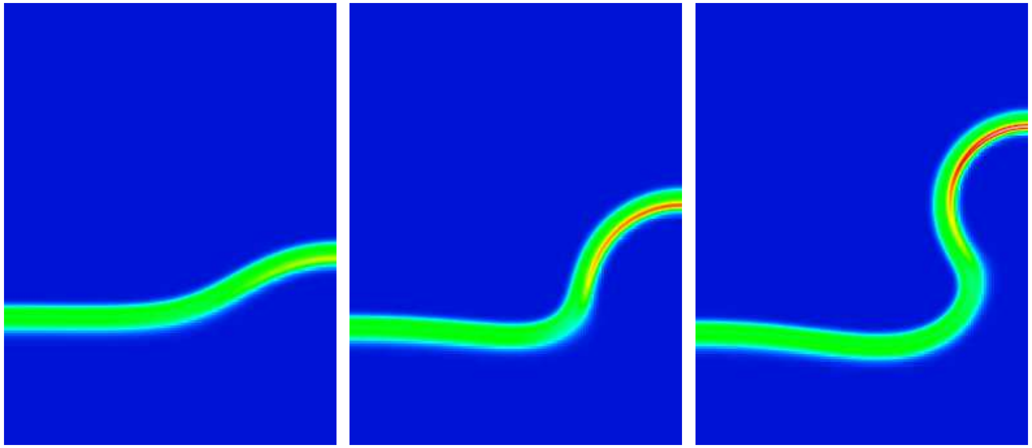




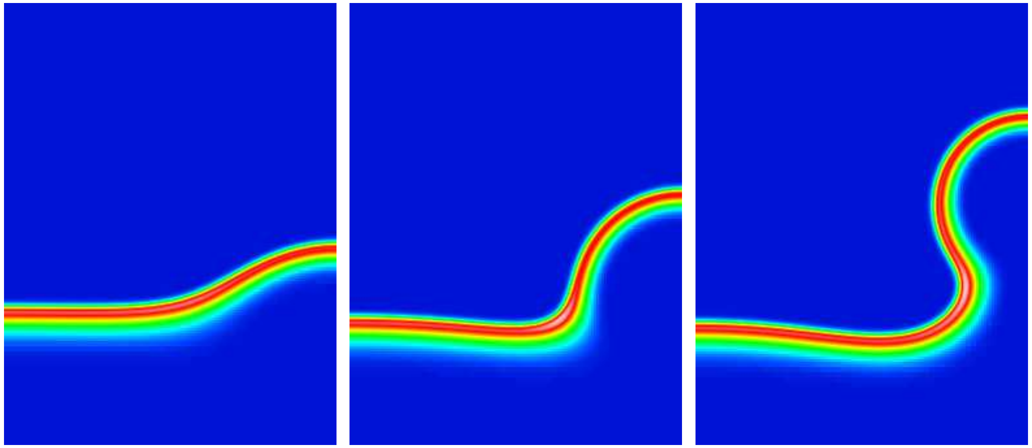
- Fuel: N_2-diluted CH_4/air
  - $\phi = 0.8$
- Mech: GRI-Mech 1.2
  - 32 species, 177 reactions

Representative adaptive solution

Chemical behavior in VFI



CH_3O enhanced where $\kappa < 0$



C_2H_4 enhanced where $\kappa > 0$

Turbulence flame sheet

Three-dimensional isotropic turbulence propagating into a premixed flame

- Tanahashi, et al (2000, 2002) Hydrogen, DNS
- Bell, et al (2002) Methane, low Mach

Flame:

- $\phi = 0.8$
- $\delta_L = 0.53$mm
- $S_L = 25$cm/s

Turbulence:

- $\ell_t = 1.0$mm
- $u'/S_L = 1.7, 4.3$

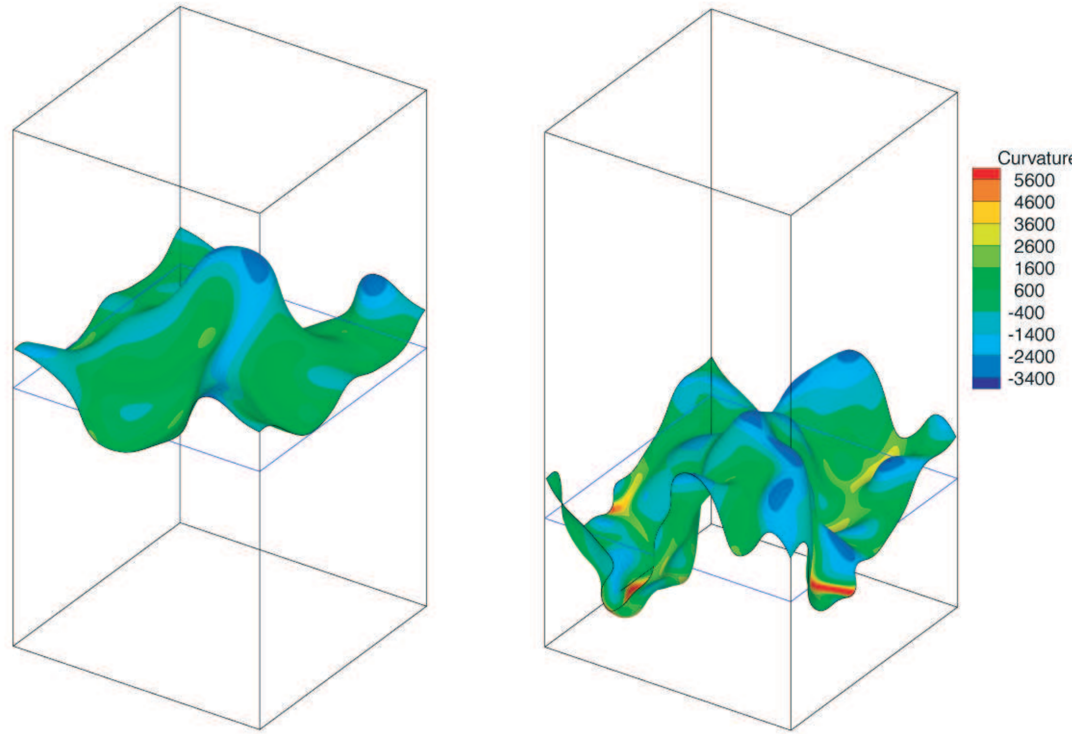
Computations:

- 8×8×16 mm domain
- doubly periodic
- $\Delta x_{\text{eff}} = 62.5\mu$m

Model:

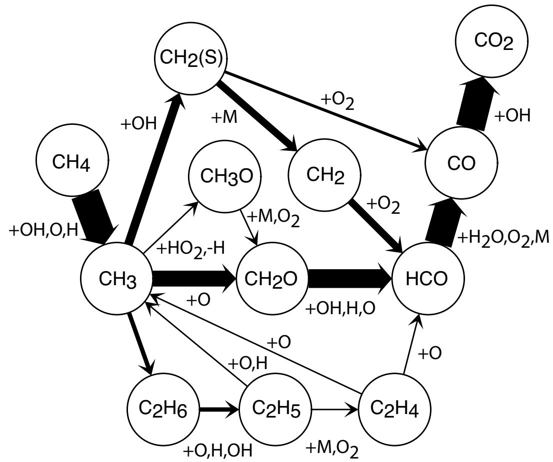
- DRM-19
- 20 species/84 reacs

$T = 1500K$ surfaces, colored by mean curvature.

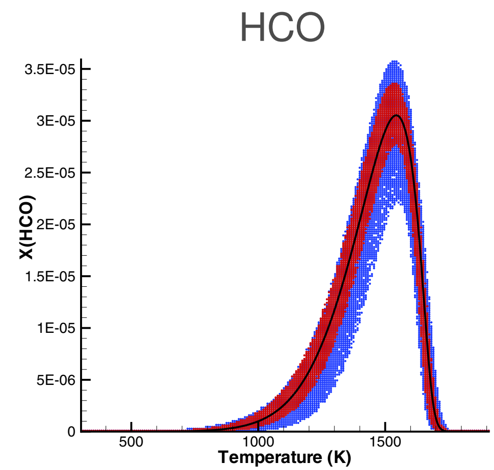


$u'/S_L = 1.7$ $u'/S_L = 4.3$

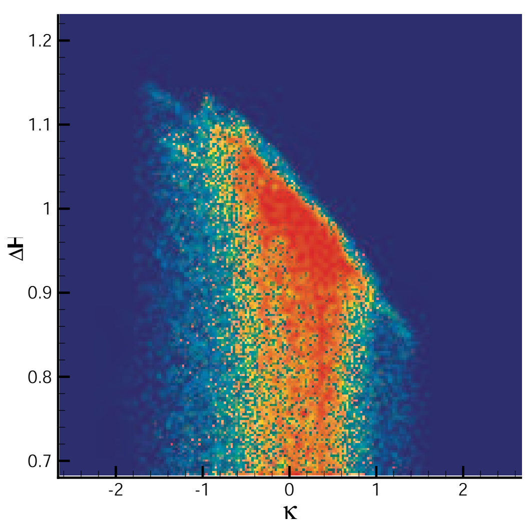
Heat Release and Flame Curvature



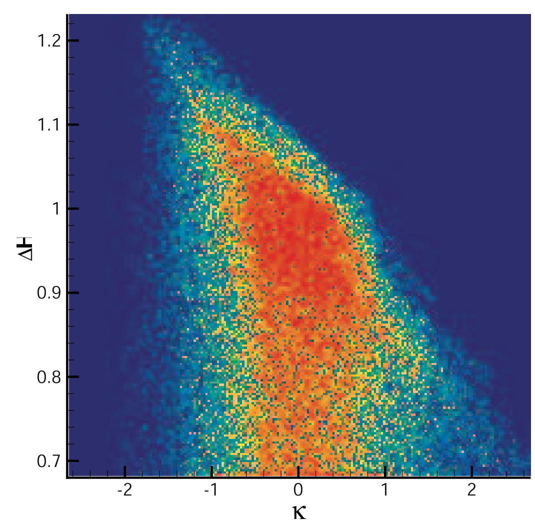
Carbon Flow Network



$U' = 1.7S_L$



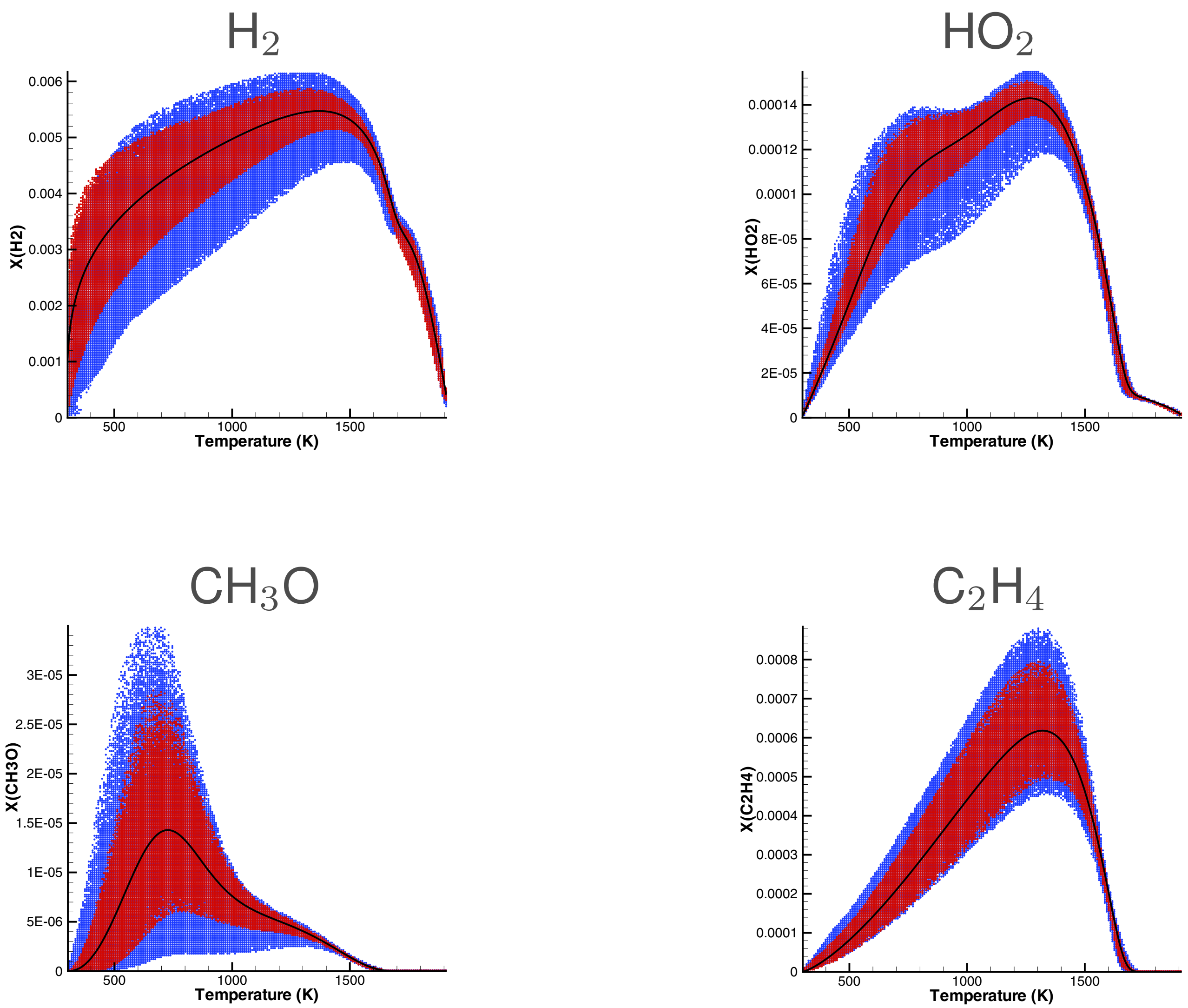
$U' = 4.3S_L$



Heat release vs. Curvature

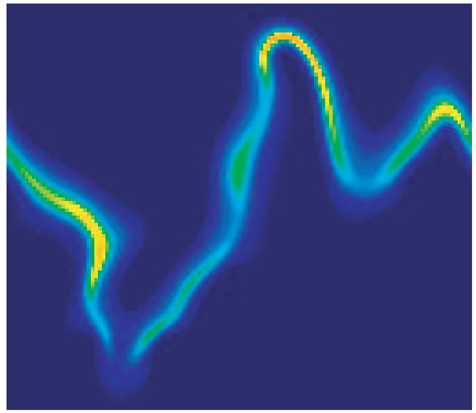
(ΔH, κ normalized by ΔH_L, δ_L)

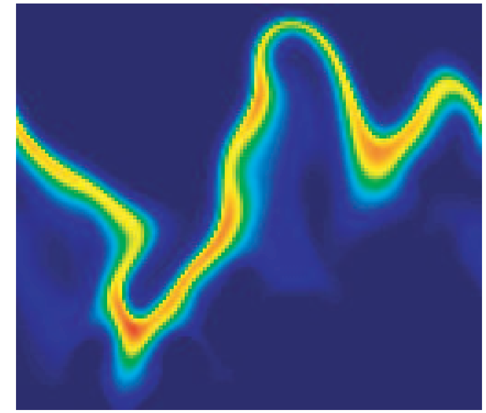
Redistribution of Species

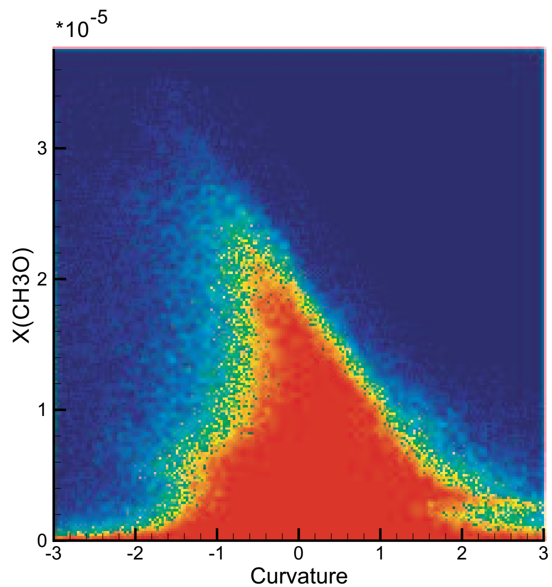


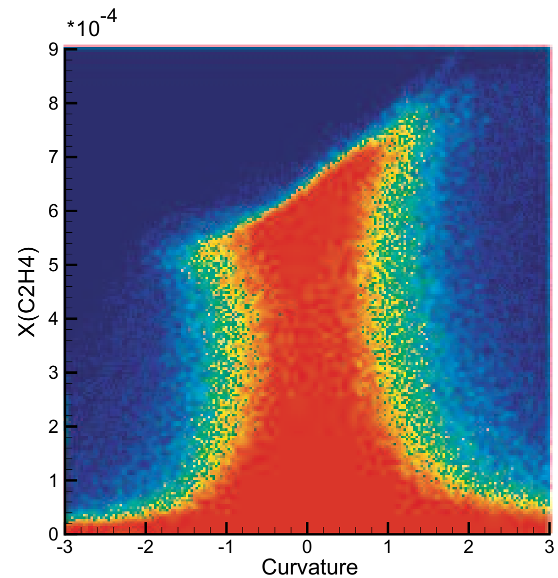
Turbulence chemistry interaction

CH_3O C_2H_4









Species concentration versus flame curvature

Full-scale Simulations

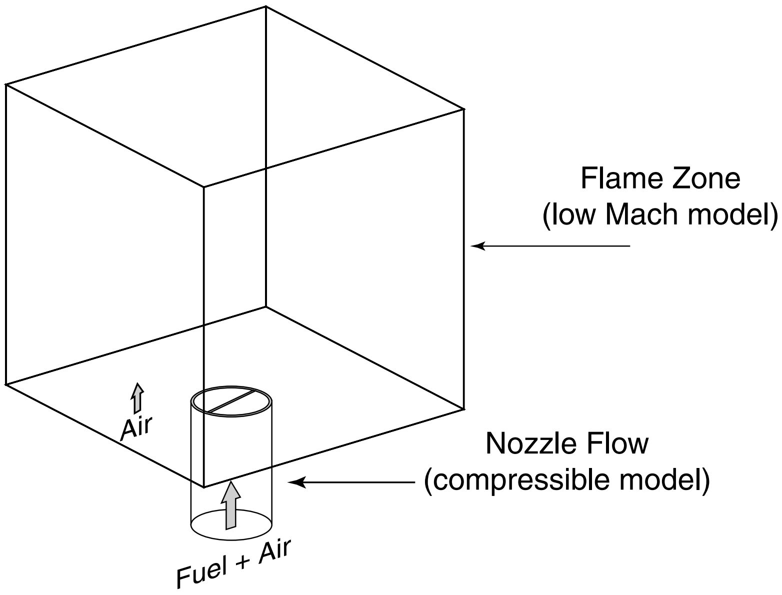
Strategy - Use compressible simulations to characterize nozzle flow

Compressible simulations of nozzle:

- Compressible effects are important in nozzle with swirl
- Provide inflow to 3-D low Mach number model

Low Mach number inflow boundary

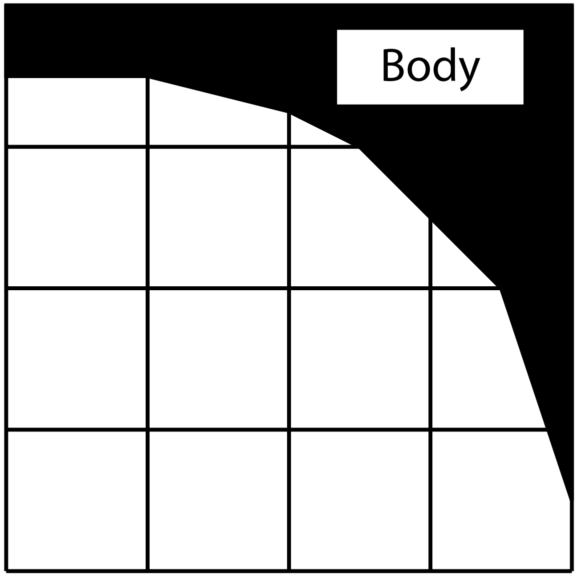
- Direct coupling to compressible solver
- Use statistics



Compressible Flow with Geometry

Model geometry as front embedded in regular Cartesian grid

- Volume fractions
- Area Fractions



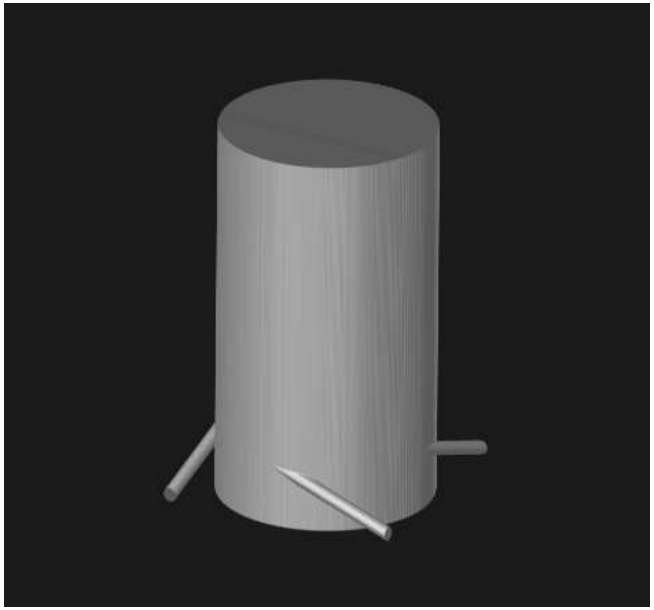
Finite volume discretization (Chern and Colella)

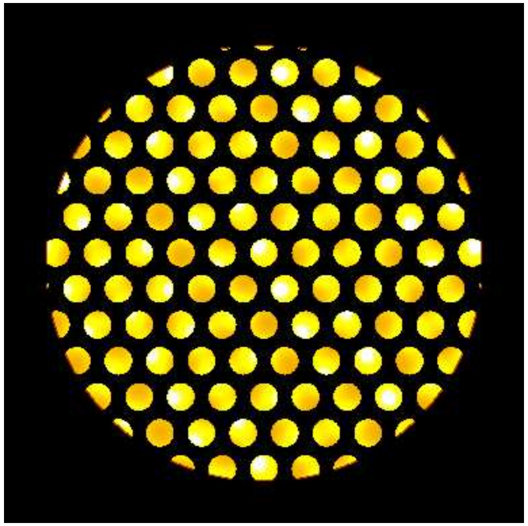
- Conservative update unstable in small cells
- Update with stable fraction
- Distribute remainder to neighboring cells

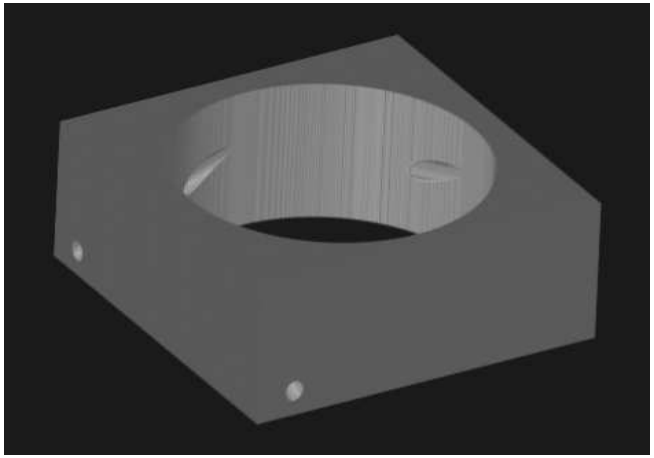
Adaptive, parallel, 3D, ...

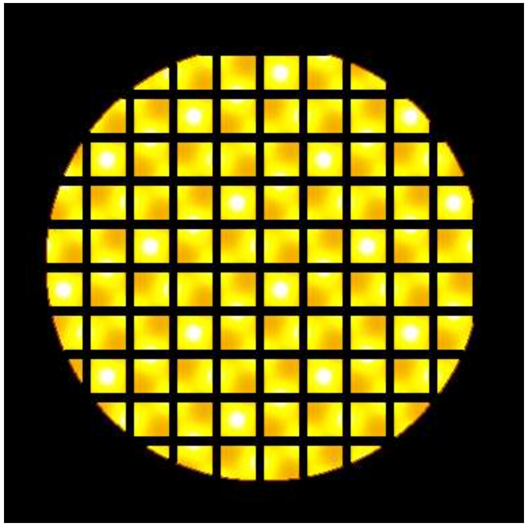
Pember et al., JCP, 1995

Nozzle Geometry

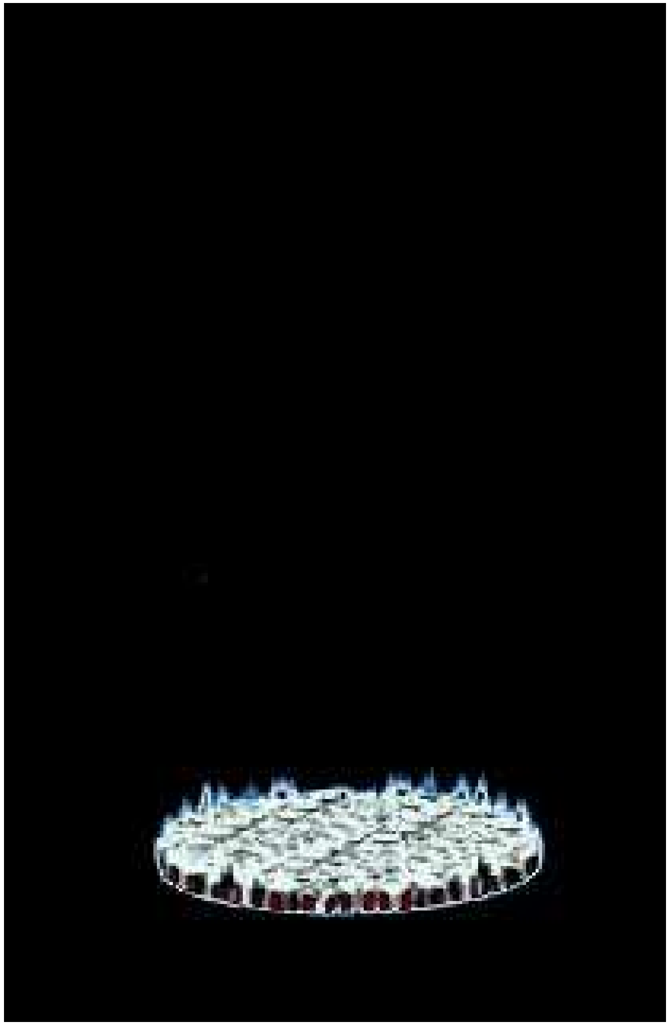




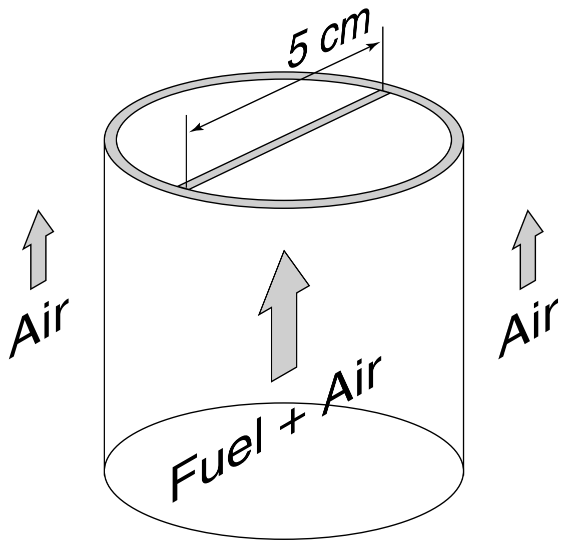


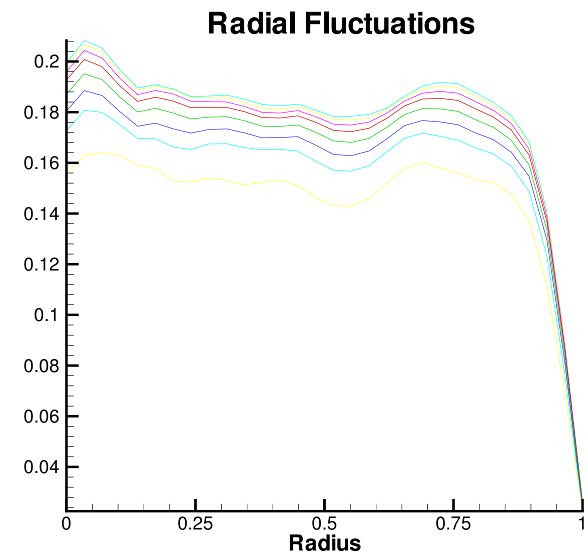


Nozzle Simulations

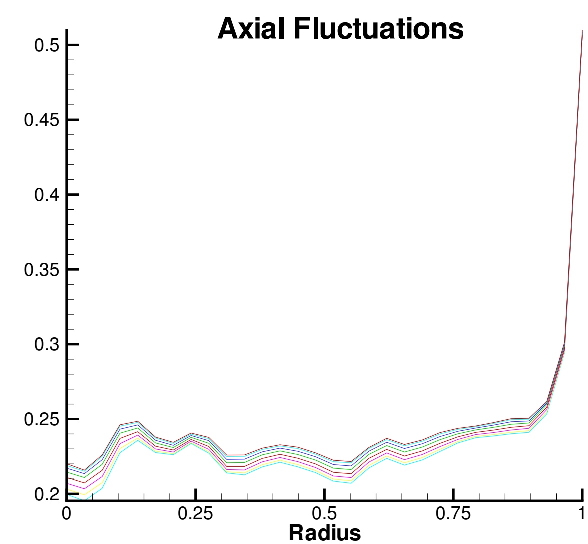


V-flame Setup



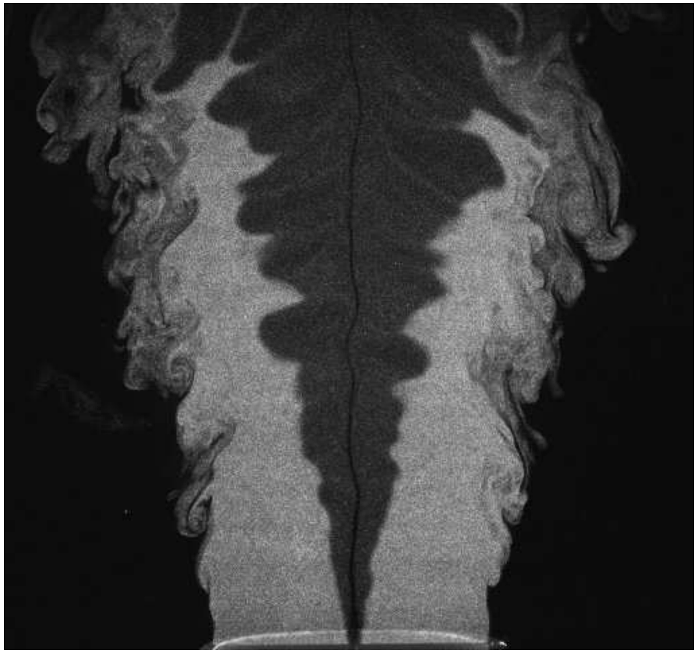


- Domain: 12cm x 12cm x 12cm
- DRM-19: 21 species, 84 reactions
- Mixture model for differential diffusion
- $\ell_t = 3.5mm$
- 3 m/s mean inflow



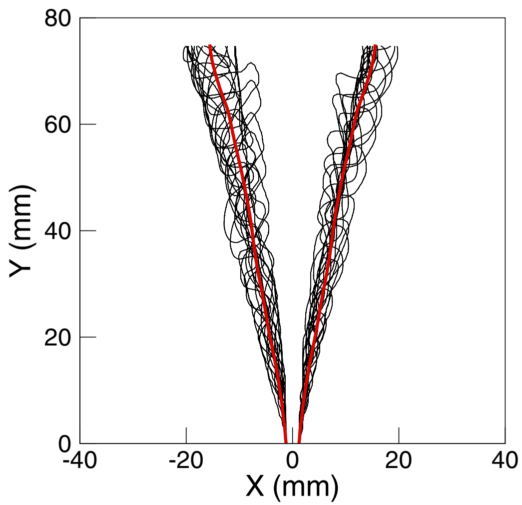
Results: Computation vs. Experiment

CH_4 from simulation

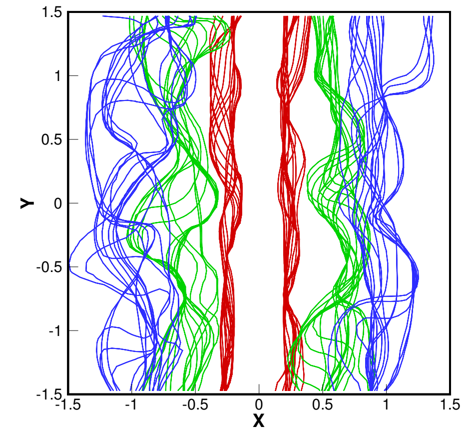


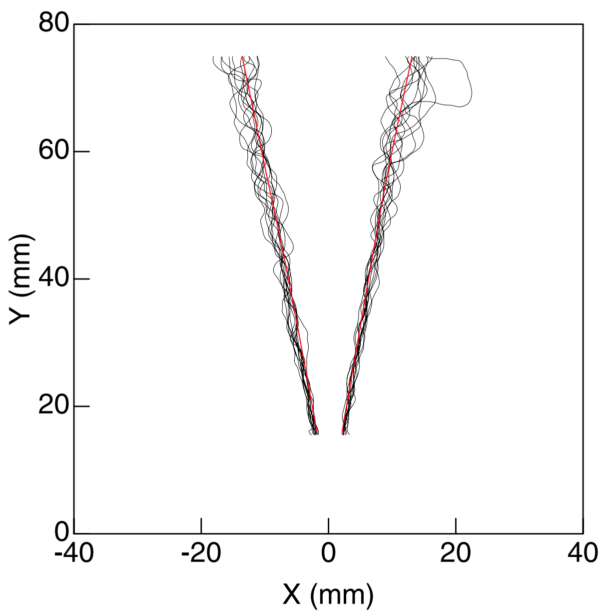
Single image from experimental PIV

Further Comparisons and Analysis

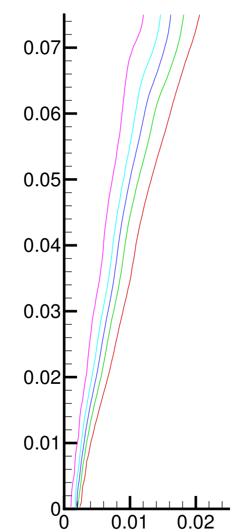


Vertical cuts – computation



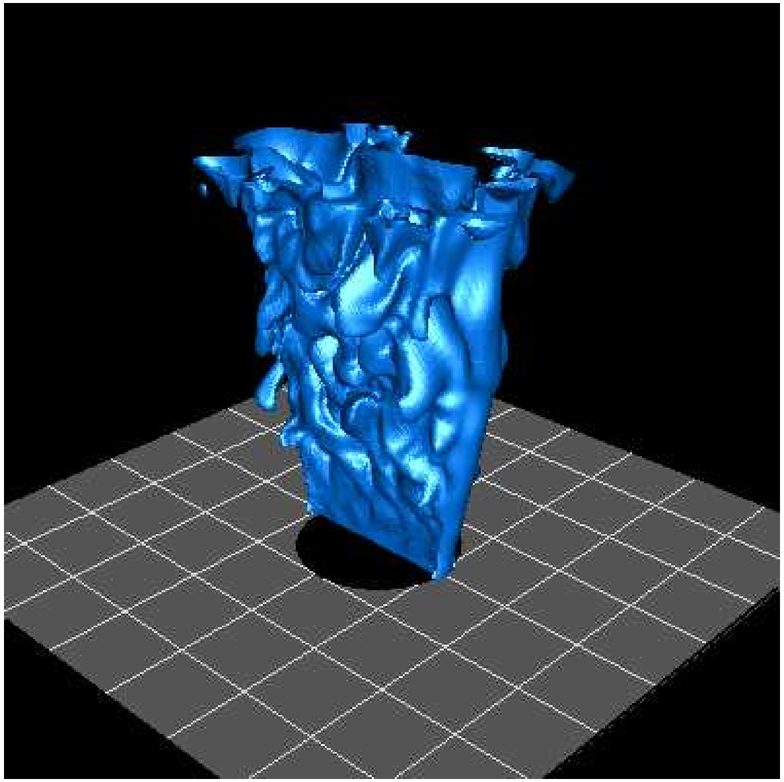


Vertical cuts – experiment



Flame brush thickness

Flame Surface



Instantaneous flame surface

Turbulent flame speed enhancement:

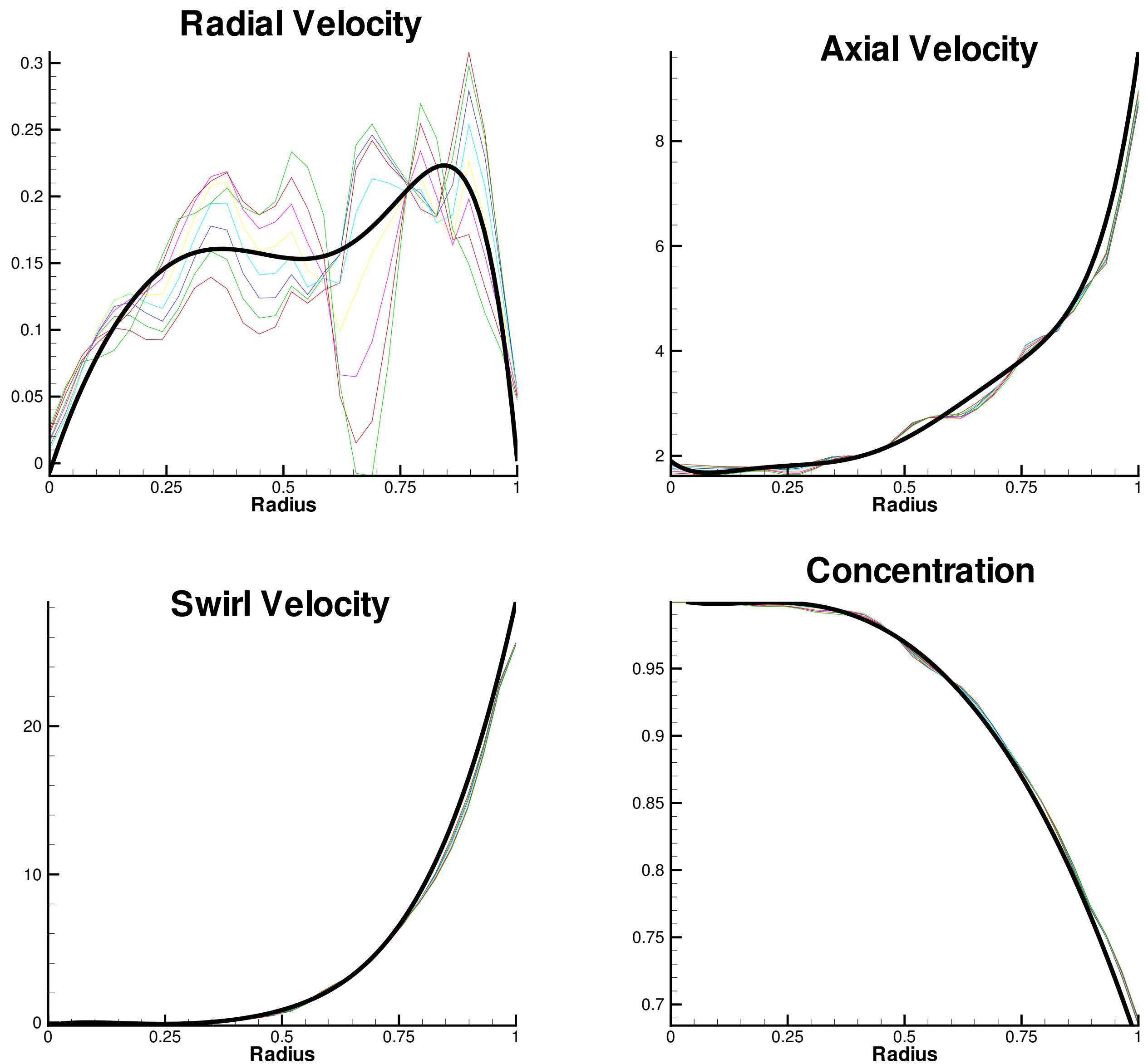
$$S_t = 1.9 S_L$$

Area enhancement due to wrinkling:

$$A_t = 1.25 A_L$$

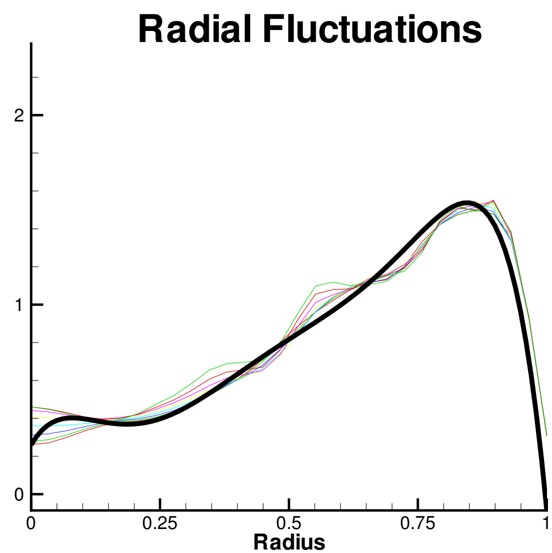
Joint with M. Johnson, R. Cheng, and I. Shepherd, EETD, LBNL

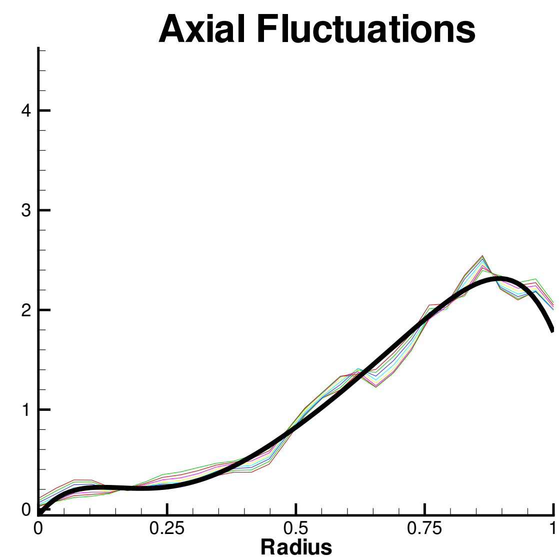
Low Swirl Burner Setup

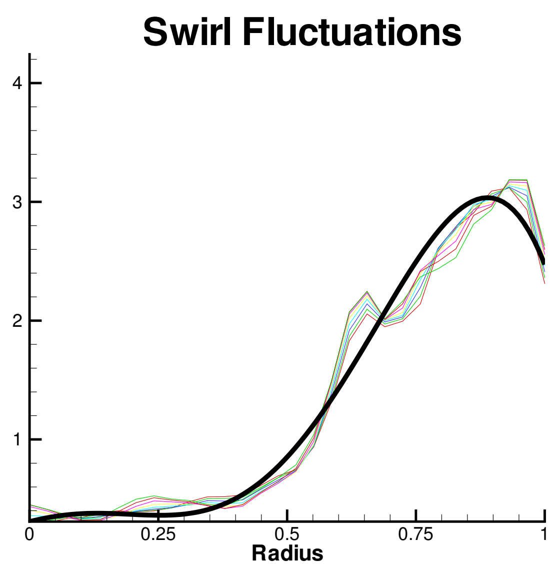


Mean profiles

Low Swirl Burner Setup



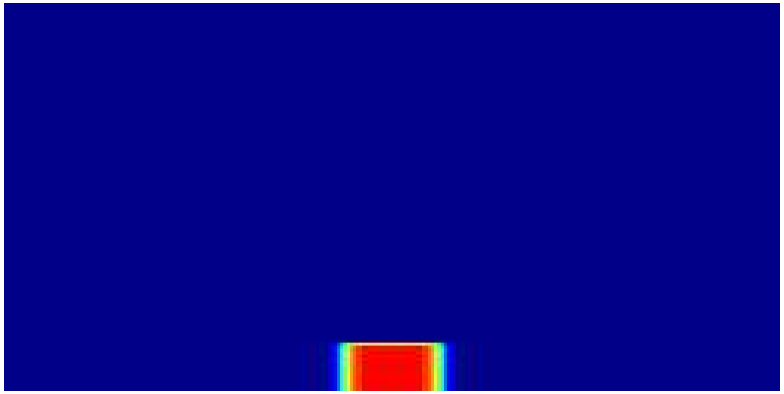




Fluctuation statistics

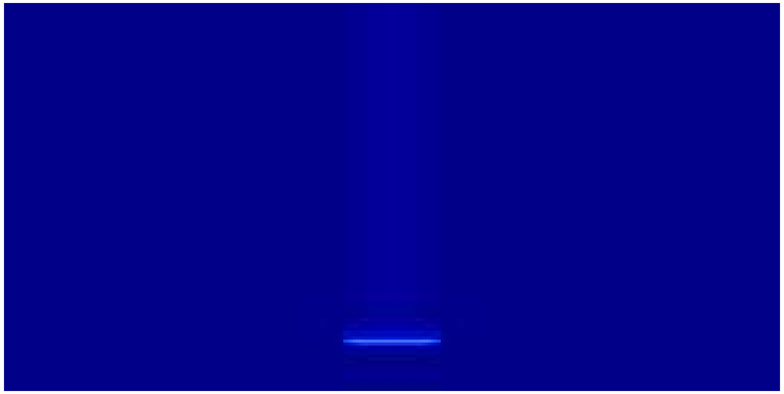
Low Swirl Burner - Preliminary Results

CH4

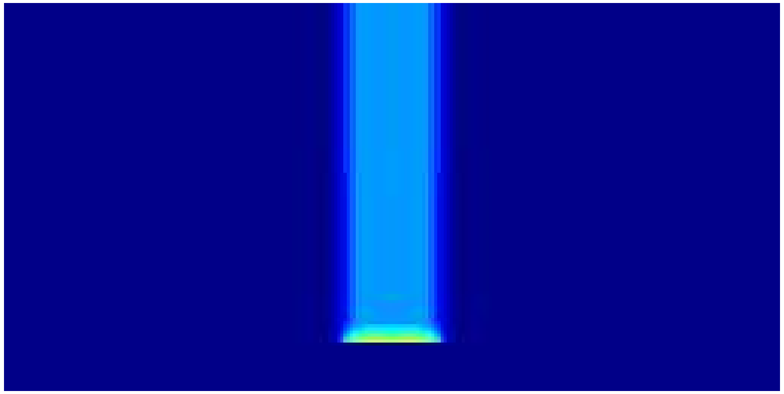


Vorticity

CO



OH



Summary and Future Work

Summary

Algorithm for low Mach number combustion

- Adaptive
- Conservative
- Second-order in time and space
- Parallel

Application to turbulent premixed combustion

- Vortex flame interaction
- 3D turbulent flame sheet
- Laboratory-scale turbulent flames

Future Work

- Futher validation / comparison with experiment
- Modeling of low swirl burner
- Characterize turbulent flame propagation properties
- Investigate turbulent flame chemistry